Finite Temperature Critical Behavior of Mutual Information

Rajiv R. P. Singh,[1] Matthew B. Hastings,[2, 3] Ann B. Kallin,[4] and Roger G. Melko[4]

[1]*Physics Department, University of California, Davis, CA, 95616*
[2]*Duke University, Department of Physics, Durham, NC, 27708*
[3]*Microsoft Research, Station Q, CNSI Building, University of California, Santa Barbara, CA, 93106*
[4]*Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada*
(Dated: March 7, 2011)

We study mutual information for Renyi entropy of arbitrary index n, in interacting quantum systems at finite-temperature critical points, using high-temperature expansion, quantum Monte Carlo simulations and scaling theory. We find that for $n > 1$, the critical behavior is manifest at two temperatures T_c and nT_c. For the XXZ model with Ising anisotropy, the coefficient of the area-law has a $t \ln t$ singularity, whereas the subleading correction from corners has a logarithmic divergence, with a coefficient related to the exact results of Cardy and Peschel. For $T < nT_c$ there is a constant term associated with broken symmetries that jumps at both T_c and nT_c, which can be understood in terms of a scaling function analogous to the boundary entropy of Affleck and Ludwig.

The numerical study of entanglement in quantum systems, through the entanglement entropy (EE) at zero temperature or mutual information (MI) at non-zero temperature, promises to be a new approach to quantifying properties of quantum phases that cannot be detected using traditional measures based on two-point correlation functions. It has already been used in one dimensional (1D) systems to identify the central charge [1, 2], in two dimensional (2D) systems to test the area law in the Heisenberg model [3, 4], and to identify a topologically ordered spin liquid phase in a 2D spin model [5].

In 1D, gapless systems described by conformal field theory show logarithmic violations of the area law [1]. However in 2D, the presence of an area law for a system such as the Heisenberg model implies that the existence of gapless modes does not necessarily lead to such a violation. Similar area-law behavior is also observed in gapless 2D bosonic theories while non-interacting fermions show a logarithmic violation [6], presumably reflecting the infinite number of gapless modes associated with the fermi surface. The question of precisely which interacting many-body models have enough entanglement to violate the area law is important both for identifying new phases and for developing novel computational tools.

Even with an area law, subleading corrections to the entanglement entropy, such as those associated with corners, can show logarithmic divergence at quantum critical points [7, 8]. While entanglement entropy at $T = 0$ remains a key focus of current research, MI at non-zero temperature (which reduces to EE at $T = 0$) can also show universal critical behavior and has been a subject of both theoretical and computational [9] studies.

From a computational point of view, there is a clear need for new methods capable of studying EE or MI for large-scale quantum systems in $D > 1$. In this paper, we develop a High Temperature Expansion (HTE) method for calculating MI for Renyi entropy of arbitrary index n for lattice models in the thermodynamic limit. Our work represents a new direction in the use of series expansions to study boundary phenomena in critical systems, enabling one to calculate corner exponents such as Cardy-Peschel exponents in 2D systems [10].

In the following, we combine HTE with quantum Monte Carlo (QMC) simulations and a scaling theory to obtain the critical behavior of MI for a 2D spin-1/2 XXZ model, $\mathcal{H} = \sum_{\langle i,j \rangle}(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z)$, with Ising anisotropy $\Delta = 4$. Quite generally, we find that for $n > 1$, the critical behavior manifests itself at two different temperatures T_c and nT_c. Since this model is in the universality class of the 2D Ising model, the singularity of the area-law term is known to be $t \ln t$, where the reduced temperature t is $|T - T_c|$ or $|T - nT_c|$, and the logarithmic divergence of the subleading corner terms can be related to the work of Cardy and Peschel [10]. We also find that spontaneously broken symmetries lead to a constant term in the MI that jumps at nT_c and T_c, described by a scaling function analogous to the boundary entropy of Affleck and Ludwig [11].

Replica Calculation of MI— Consider a system divided into two regions A and B, where ρ_A is the reduced density matrix on A. The Renyi entropies are defined as

$$S_n(\rho_A) = \frac{1}{1-n} \ln \left[\text{Tr}(\rho_A^n) \right]. \tag{1}$$

The von Neumann entropy S_1 is defined by the limit $n \to 1$. The advantage of the $n > 1$ Renyi entropies is that they can be calculated by a "replica method" for integer n [1], where for a given inverse temperature β, one must evaluate a partition function $Z[A, n, T]$ corresponding to a path integral on a system with modified space-time topology. In region A, the system is periodic with period $n\beta$, while in region B there are n distinct sheets, each periodic with period β. Normalizing correctly, one has,

$$\text{Tr}(\rho_A^n) = \frac{Z[A, n, T]}{Z[T]^n}, \tag{2}$$

where $Z[T]$ denotes the partition function at temperature T. This replica method was used in [9] for QMC simulations of S_2. In this paper, we perform similar simulations
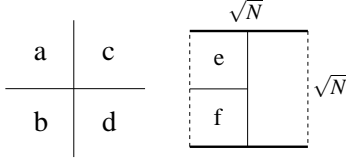
FIG. 1: In the HTE (left), we consider partitions of the infinite square-plane where region A could be a half-plane such as $a \cup b$ or a quadrant such as b or c. In QMC (right) the N-site real space lattice is a torus with periodic boundaries, or a cylinder with the dashed boundaries open. In the torus, region A can be e ("square") or $e \cup f$ ("strip"), while for the cylindrical we use a strip ($e \cup f$) region A.

(for $n = 2$ and higher) and also develop a HTE method to calculate the partition function with this modified topology in powers of β. We are interested in determining the MI between region A and its complement B, defined as

$$I_n = S_n(\rho_A) + S_n(\rho_B) - S_n(\rho). \qquad (3)$$

One important feature of this calculation is that if the given Hamiltonian has a critical point at temperature T_c, then the partition function $Z[A, n, T]$ shows critical behavior at $T = nT_c$ because the path integral is periodic with period $n\beta$ in region A. If we consider a semi-infinite region A (for example, dividing a 2D plane into two half-planes) then $Z[A, n, T]$ will be non-analytic at $T = nT_c$. In contrast, the von Neumann MI, I_1, should not show critical behavior at temperatures other than T_c.

High Temperature Series and MI— We develop a HTE for the MI in powers of $\beta = 1/T$. One important simplification of MI is that all terms proportional to the volume of A, B cancel out and we are left with only terms localized near the boundary of A, B. The reason for this is that a given bulk term in region A appears once at temperature T/n in $Z[A, n, T]$ but also appears once at temperature T/n in $Z[T/n]$ – these cancel out. Similarly, this term appears n times in $Z[B, n, T]$ but also appears n times in $n \ln(Z[T])$.

The HTE is calculated by a linked cluster method [12, 13]. We imagine that the infinite system is divided into subregions A and B either by a single straight line running parallel to one of the axes, or by two perpendicular lines that meet at a point (Fig. 1). The line contribution to the MI is obtained by considering region A to be the half-plane $a \cup b$. To obtain the corner contribution we consider four separate partitions of the square lattice: the region A can be (i) the quadrant b (ii) the quadrant c (iii) the half-plane $a \cup b$ or (iv) the half plane $a \cup c$. If we add MI from the first two partitions and subtract those from the next two, all line contributions cancel. The difference defines two times the contribution from a single corner. More generally, we express I_n as

$$I_n = a_n(\beta) \cdot L + n_c b_n(\beta) + d_n(\beta), \qquad (4)$$

TABLE I: High temperature series coefficients for the line and corner terms for Renyi MI for $n = 2$.

m	l_m	f_m
2	1.125	0
3	0.375	0
4	6.32421875	-2.765625
5	-5.109375	0.46875
6	64.02701823	-27.11848958
7	15.59501953	-0.3969401042
8	1079.586016	-584.0700043
9	97.15596924	-63.38234592
10	12847.34193	-8700.183385
11	-1079.890682	94.58389488

where a_n, b_n, d_n depend on β, L is the length of the boundary, n_c is number of corners, and d_n is a constant term, associated with symmetry breaking, to be explained later.

Before division by the factor $(1 - n)$, the coefficient of β^m is a polynomial in n of order m, which vanishes at $n = 0$ and $n = 1$. Thus dividing by $1 - n$ and taking the limit $n \to 1$ is simple and reduces the final coefficient to a polynomial of order $m - 1$. The complete expression for the line term to β^4 is:

$$
\begin{aligned}
a_n(\beta) &= \left(\frac{\beta}{4}\right)^2 \frac{nA_2}{2} - \left(\frac{\beta}{4}\right)^3 \frac{n(n+1)A_3}{6} \\
&\quad + \left(\frac{\beta}{4}\right)^4 \left[n(n^2 + n + 1)\left(\frac{A_4}{24} - \frac{A_2^2}{8}\right) \right. \\
&\quad \left. + n(n^2 + n - 1)\left(\frac{B_4 - A_2^2}{2} + C_4\right) \right]. \quad (5)
\end{aligned}
$$

Here, $A_2 = 2 + \Delta^2$, $A_3 = -6\Delta$, $A_4 = (2 + \Delta^2)^2 + 4(1 + 2\Delta^2)$, $B_4 = \Delta^4 - 4\Delta^2$ and $C_4 = 2 + \Delta^4$. In addition, we have calculated both the line and corner contribution for the second Renyi entropy up to order β^{11}. Let

$$a_2(\beta) = \sum_m l_m \beta^m, \qquad b_2(\beta) = \sum_m f_m \beta^m. \qquad (6)$$

The coefficients l_m and f_m up to $m = 11$ for the second Renyi entropy for $\Delta = 4$ are given in Table I.

Comparison with Exact Numerics – We calculate the MI via exact diagonalization (ED), and Stochastic Series Expansion [14] QMC using the replica-trick, Eq. (2). We extend the QMC algorithm outlined in Ref. [9] to allow calculations to arbitrary Renyi entropies by directly constructing a simulation cell with n sheets [16]. Geometries considered are illustrated in Fig. 1. The critical temperature of the model is best determined by studying the Binder ratios associated with the order parameter. We estimate $2.234 < T_c < 2.237$, which gives $\beta_c/2$ in the range 0.2235 to 0.2238.
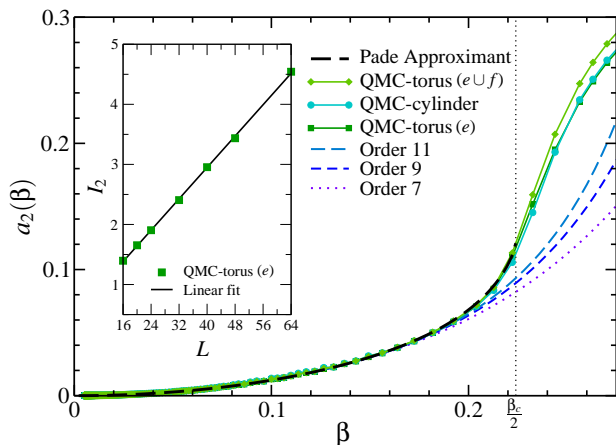
FIG. 2: (color online) A comparison of MI calculated with HTE, and QMC on 32×32 simulation cells on toroid and cylindrical geometries (see Fig. 1). Inset: MI plotted against L at $\beta = 0.204$, showing excellent fit to linear form.

FIG. 3: (color online) MI divided by boundary length from the fourth-order series expansion for: I_1, compared to ED on a 4×4 system with 3×3 region A; and I_4, compared to QMC for 10×10 and 20×20. A sharp change in slope in I_4/L occurs at $1/4T_c$, where $T_c = 2.24$, obtained from the crossing of the fourth-order Binder cumulant for the staggered magnetization. Inset: the constant scaling term d_4 extracted from a linear fit to the QMC data.

Fig. 2, shows the partial sums of the 11-th order series for the linear terms (area-law) for $n = 2$ compared with QMC data. One can see that the results agree extremely well up to a β value of 0.21, at which point the QMC data shows a sharp rise. To study the critical behavior more closely we use Pade approximants. The 2D Ising universality class is special in that the correlation length exponent $\nu = 1$ and the boundary free energy has a $t \ln t$ singularity [15]. Anticipating this, we take two derivatives of the series, and use Pade approximants biased to have a pole at the $\beta_c/2$ value obtained from the Binder ratios. Upon integration, these lead to a $t \ln t$ singularity. One such approximant is shown in Fig. 2 (thick dashed line). It captures the sharp rise in QMC data extremely well, confirming the $t \ln t$ behavior to high accuracy.

The corner terms should have a logarithmic singularity. In fact, the series for $db_2/d\beta$ show good convergence for a simple pole implying that b_2 goes as some constant x times $\ln t$. To get an accurate estimate for the coefficient x, we once again bias the critical temperature values. With the critical point biased at 0.223 the spread of Pade approximants leads to an estimate of $x = 0.0143 \pm 0.0013$, where as biasing it at 0.224 leads to an estimate of 0.0151 ± 0.0016. We can relate these coefficients to the exact results of Cardy and Peschel [10]. The internal angle for the corner is $\gamma = \pi/2$ for region A and $\gamma = 3\pi/2$ for region B. Together with $c = 1/2$ for the Ising model, Eq. 4 in Ref. [10] leads to a $-\frac{1}{72} \ln L$ singularity at the critical point. This, using $\nu = 1$, translates in to an x value of $\frac{1}{72} = 0.013\bar{8}$. Our results show that for exactly soluble 2D universality classes with known values of the central charge, the results of Cardy and Peschel can be used to obtain the coefficient x.

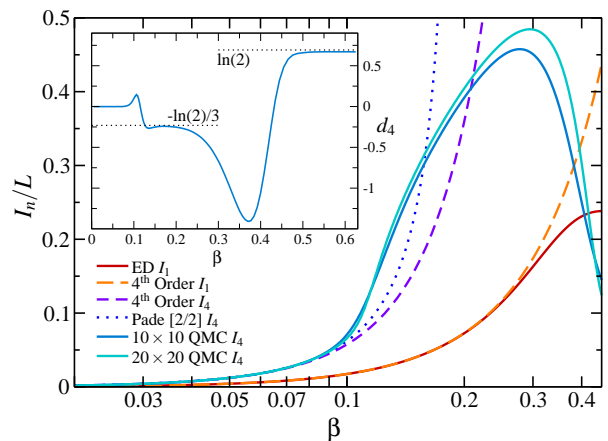Fig. 3 shows a comparison of the von Neumann MI, calculated by continuing the HTE to $n = 1$, with results

obtained by exact diagonalization (ED) on a 4×4 system. In this case, we have multiplied the series by the length of the boundary separating regions A and B. The agreement is excellent up to $\beta \approx 0.25$, which confirms the validity of both calculations and shows that finite size effects are small at smaller β values. The von Neumann entropy series should be convergent down to T_c. Fig. 3 also compares HTE and QMC simulation results for I_4, which further confirms that for I_n the higher temperature singularity moves to nT_c. The inset illustrates the constant scaling term $d_4(\beta)$ extracted from QMC data taken on 10×10 and 20×20 toroidal simulation cells with strip regions A ($e \cup f$ in Fig. 1). At low temperatures, $d_4(\beta)$ approaches the value $\ln(2)$ predicted from our scaling theory. For temperatures between T_c and nT_c, theory predicts that $d_n = -\ln(2)/(n-1)$, discussed below, which is visible as a plateau in the QMC data.

Constant Terms in the MI Due to Symmetry Breaking— We now consider the MI between region A and B away from criticality, in the limit of large system size. In addition to the line and corner terms, symmetry breaking can lead to additional constant terms d_n. First, consider the case of $T < T_c$, where the Ising symmetry is broken in all regions. The breaking of the symmetry means that the partition functions $Z[T], Z[T/n], Z[A,T,n], Z[B,T,n]$ all have a multiplicative factor of 2 in addition to the volume, line, and corner terms. The volume terms still cancel, and the line and corner terms still contribute according to Eq. (4), but the factors of 2 increase the MI by $\ln(2)$. Similarly, for $T_c < T < nT_c$, the partition function $Z(T)$ has no additional factors of 2 but $Z(A, n, T), Z(B, n, T)$

and $Z(T/n)$ do, giving rise to a constant term in MI of $d_n = -\ln(2)/(n-1)$. These are verified by the plateau in the QMC data in the inset of Fig. 3. These results are modified strongly by finite size effects due to the volume terms which go generically as $\exp(-L/\xi)$, but can be substantial when ξ is comparable to or larger than L. These form part of the scaling theory, which we develop next.

Scaling Theory Near nT_c — Near $T = nT_c$ we can use scaling theory to describe the singular behavior of the Renyi entropy. The sheets of the system with period β are not critical, while the region with period $n\beta$ is in a critical scaling regime. Consider first the case that $T > nT_c$ and $L \gg \xi$. Then, we can calculate the MI by using a scaling ansatz for the free energy of a critical theory with a boundary, which implies that the singular terms in the MI equal $c_1(L/\xi) + c_2 n_c \ln(\xi)$ for some universal constants c_1, c_2. The c_1 term represents the fact that the singular terms in the MI are due to degrees of freedom at length scale ξ and there are L/ξ such terms. For $T < nT_c$ and $L \gg \xi$, there is the additional $-\ln(2)/(n-1)$ described above, but the singular MI behaves again as $c_1'(L/\xi) + c_2 n_c \ln(\xi)$. For $L \sim \xi$, finite size scaling implies that the MI is equal to $F(Lt^\nu) + n_c \ln(\min(L, \xi))$ plus smooth terms (such smooth terms multiplying L or n_c) where $F(x) \to c_1 x$ as $x \to +\infty$, $F(x) \to c_1'|x| - \ln(2)/(n-1)$ as $x \to -\infty$. At $x = 0$, $F(x)$ equals n times the Affleck-Ludwig boundary entropy [11].

The 2D Ising universality class with $\nu = 1$ is special and in this case the line term has a multiplicative log correction as verified in our series analysis. The subleading corner term is predicted to diverge logarithmically, in agreement with the series calculation. The negative jump in the additive constant term together with an increasing line term leads to an approximate crossing of I_n/L for different system sizes near nT_c as seen in the QMC data in Fig. 3.

Scaling Theory at T_c — At T near T_c, we can again develop a scaling theory. In contrast to the case of $T \approx nT_c$, the region with period $n\beta$ is now in the ordered phase, and the n sheets with period β display critical scaling of a theory with a boundary magnetization (since the region with period $n\beta$ is ordered). For $L \gg \xi$, the singular terms in the MI again behave as $c_3(L/\xi) + c_4 n_c \ln(\xi) - \ln(2)/(n-1)$ or $c_3'(L/\xi) + c_4 n_c \ln(\xi) + \ln(2)$ depending on whether $T > T_c$ or $T < T_c$ with universal constants c_3, c_3', c_4. The change in sign in the constant from $-\ln(2)/(n-1)$ to $\ln(2)$ leads to a crossing of I_n/L for different system sizes at T_c (with corrections from line and corner terms which shift the crossings at finite L to larger T). There is again a multiplicative log correction in the Ising case. This critical point corresponds to the case of a boundary magnetic field, while the $T = nT_c$ critical point corresponds to the case of free boundary conditions – but both produce a log correction.

Discussion — We have developed computational methods and scaling theory to study Renyi mutual information I_n in interacting quantum systems. Away from critical points the MI consists of line terms (area-law), corner terms, and constant terms coming from symmetry-breaking. At the critical points the line terms develop a singularity which vanishes as $1/\xi$, and thus have a critical exponent ν. In the special case of the 2D Ising universality class with $\nu = 1$, there are multiplicative log terms. The subleading corner terms show a log divergence, whose coefficient can be related to the central charge using the results of Cardy and Peschel [10]. We also find that the constant terms jump discontinuously at the transitions and can be described by a scaling function that is analogous to the boundary entropy of Affleck and Ludwig [11].

We have extended our previous QMC algorithm for I_2 [9] to calculate arbitrary I_n by using a multi-sheeted space-time simulation cell, and confirmed the main results of the scaling theory. QMC methods are able to access all temperature regions, allowing one to obtain the bulk terms due to symmetry breaking. HTE can separately obtain the line terms and subdominant corner terms. Since the HTE is immune to the sign problem, it should be a general tool for calculating MI in arbitrary interacting quantum systems such as frustrated spin or fermionic models in the future.

[1] P. Calabrese and J. Cardy, J. Stat. Mech.: Theor. Exp. **P06002** (2004).

[2] A. Feiguin, S. Trebst, A. W. W. Ludwig, M. Troyer, A. Kitaev, Z. Wang, and M. H. Freedman, Phys. Rev. Lett. **98**, 160409 (2007).

[3] A. B. Kallin, I. González, M. B. Hastings, and R. G. Melko, Phys. Rev. Lett. **103**, 117203 (2009).

[4] M. B. Hastings, I. González, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett. **104**, 157201 (2010).

[5] S. Isakov, M. B. Hastings, and R. G. Melko, arXiv:1102.1721 (2011).

[6] M. Cramer, J. Eisert, and M. B. Plenio, Phys. Rev. Lett. **98**, 220603 (2007).

[7] H. Casini and M. Huerta, Nucl. Phys. B **764**, 183 (2007).

[8] T. Nishioka, S. Ryu, and T. Takayanagi, J. Phys. A **42**, 504008 (2009).

[9] R. G. Melko, A. B. Kallin, and M. B. Hastings, Phys. Rev. B **82**, 100409 (2010).

[10] J. L. Cardy and I. Peschel, Nuclear Physics B **300**, 377 (1988).

[11] I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).

[12] J. Oitmaa, C. J. Hamer, and W. Zheng, *Series Expansion*

Methods for Strongly Interacting Lattice Models (Cambridge University Press, 2006).

[13] M. P. Gelfand, R. R. P. Singh, and D. A. Huse, J. Stat. Phys. **59**, 1093 (1990).

[14] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991); A. W. Sandvik, J. Phys. A **25**, 3667 (1992).

[15] H. Au-Yang and M. E. Fisher, Phys. Rev. B **11**, 3469 (1975).

[16] We use a consistent energy normalization which does not include n, e.g. in Eq. (8) of Ref. [9].